PB86-130036

Theoretical Model of Soiling of Surfaces by Airborne Particles

(U.S.) Environmental Protection Agency
Research Triangle Park, NC

Nov 85

U.S. Department of Commerce
National Technical Information Service
NTIS

PB86-130036

EPA/600/D-85/279
November 1985

THEORETICAL MODEL OF SOILING OF SURFACES BY AIRBORNE PARTICLES

Fred H. Haynie
Atmospheric Sciences Research Laboratory
Office of Research and Development
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711

ATMOSPHERIC SCIENCES RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
RESEARCH TRIANGLE PARK, NC 27711

REPRODUCED BY
NATIONAL TECHNICAL
INFORMATION SERVICE
U.S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

TECHNICAL REPORT DATA (Please read Instructions on the reverse before completing)		
1. REPORT NO. EPA/600/D-85/279	2.	3. RECIPIENT'S ACCESSION NO. PB86 130036/AS
4. TITLE AND SUBTITLE THEORETICAL MODEL OF SOILING OF SURFACES BY AIRBORNE PARTICLES		5. REPORT DATE November 1985 6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) Fred H. Haynie		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS (Same as Box 12)		10. PROGRAM ELEMENT NO. CDTA1D/06-0015 (FY85) 11. CONTRACT/GRANT NO.
12. SPONSORING AGENCY NAME AND ADDRESS Atmospheric Sciences Research Laboratory - RTP, NC Office of Research and Development U.S. Environmental Protection Agency Research Triangle Park, North Carolina 27711		13. TYPE OF REPORT AND PERIOD COVERED 14. SPONSORING AGENCY CODE EPA/600/09
15. SUPPLEMENTARY NOTES		

16. ABSTRACT

A model is developed which can be used to predict the change in reflectance from a surface as a function of time. Reflectance change is a measure of soiling caused by the deposition of particles on a surface. The major inputs to the model are the parameters to a bimodal distribution of ambient particle concentration, surface roughness, friction velocity, particle and substrate reflectance, and whether the surface is vertical or horizontal. A new model for deposition velocity was developed for rough surfaces using Reynold's number - friction factor data and available particle deposition data.

The model is used to demonstrate the effects of changing input parameters on rates of soiling of surfaces.

17. KEY WORDS AND DOCUMENT ANALYSIS		
a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
18. DISTRIBUTION STATEMENT RELEASE TO PUBLIC	19. SECURITY CLASS (This Report) UNCLASSIFIED	21. NO. OF PAGES 23
	20. SECURITY CLASS (This page) UNCLASSIFIED	22. PRICE $9.95

EPA Form 2220-1 (Rev. 4-77) PREVIOUS EDITION IS OBSOLETE

NOTICE

This document has been reviewed in accordance with U.S. Environmental Protection Agency policy and approved for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

THEORETICAL MODEL OF SOILING OF SURFACES BY AIRBORNE PARTICLES

INTRODUCTION

The Clean Air Act calls for the review of scientific criteria every five years for those pollutants for which National Ambient Air Quality Standards have been set. Thus, standards may be revised based on the latest available evidence. Primary standards are set to protect human health with a margin of safety, without considering costs. Secondary standards are designed to protect welfare, which implies cost considerations in optimizing total benefits.

Particulate matter is one of the six ambient air quality criteria pollutants. The current secondary standard for this pollutant is 150 $\mu g/m^3$ (high volume sampler) 24 hour average not to be exceeded more than once each year. The criterion for this standard is the effect on visibility. The standard, however, also reduces soiling effects.

The most recent review of the scientific criteria has lead to the conclusion that human health can best be protected with a fine particle standard. The fine fraction also contributes the most to visibility effects. Not enough is known about soiling effects, however, to conclude that such a standard would provide significant protection from this nuisance.

This lack of knowledge prompted EPA to conduct a "Workshop on Research Strategies to Study the Soiling of Buildings and Materials" in November 1983 (1). One of the conclusions from this workshop was that theoretical studies could be done immediately, independent of other efforts, using existing data. This paper is a theoretical effort to determine the relative contribution of different size particles to the soiling of material surfaces.

THEORY

The workshop defined soiling as a surface degradation that can be undone by cleaning. It further defined a physical measure of soiling as the contrast in reflectance of particles on a substrate to the reflectance of the bare substrate. This suggests that the reflectance of a soiled surface is related to the reflectance of particles and the fraction of substrate covered by particles. A simple mathematical expression that should be applicable to particles with diameters greater than the wavelengths of light is:

$$R = R_O(1-X) + R_pX \qquad (1)$$

where R, R_O and R_p are the respective reflectances of the soiled surface, the bare substrate, and the particles collected in bulk

X is the fraction of surface covered by particles

The reflectance of particles with diameters less than the wavelength of visible light (about 0.5 μm) is expected to change with size because light interference rather than absorption becomes the dominant factor. Complete coverage ($X=1$) by very thin films may not proportionately alter the substrate reflectance because such films are not opaque.

Under constant conditions, the rate of change in fraction of surface covered will be directly proportional to the fraction of surface yet to be covered. Therefore, by integration:

$$X = 1 - \exp(-kt) \qquad (2)$$

where t is time and k is a function of particle distribution and dynamics.

Expressed mathematically:

$$k = \alpha\Sigma\, n_i u_i c_i / \rho_i r_i \qquad (3)$$

where n is the fraction of particles reaching a surface that are retained on it

u is particle deposition velocity

c is ambient concentration of particles (mass)

ρ is effective particle density

r is effective particle radius

i indicates a specific size range of particles

α is a constant based on the units selected for each parameter.

The term k has units of cross sectional area of accumulated particles per unit area of substrate surface per unit of time. For very small particles accumulated volume rather than cross sectional area coverage is probably a better indicator of soiling potential. A transition from units of area to volume units can be modelled by replacing r_i in equation (3) with

$$(r_i+0.75r_t/(r_t+r_i)) \qquad (4)$$

where r_t is the transition radius (less than 0.25μ).

When a surface is sticky or wet, all of the particles reaching the surface will be retained. Thus, as an upper limit n_i equals one for all size particles. Particles less than one micrometer generally will be retained regardless of surface condition.

Assuming that particle density ρ_i is independent of particle size should have little effect on the analysis of soiling potential of different size particles. Thus, in order to model the soiling potential (k), concentration (c_i) and deposition velocity (u_i) are the only complex particle size dependent functions that need to be expressed mathematically in this paper.

Particle Size Distribution

Ambient mass concentrations of particle sizes typically have bimodal log normal distributions (2). Thus, c_i can be mathematically expressed in terms of total concentration (C), fraction in each mode (P) and (1-P), mode diameters (D_f and D_c), and geometric standard deviations of the fine and course modes (σ_f and σ_c) (3). Dividing the particle size spectrum into intervals of one-sixth of the logarithm of decade diameter gives the following distribution:

$$c_i = 0.1531\, C\{(P/\ln(\sigma_f)) \exp(-((\ln(2r_i)-\ln(D_f))/(\sqrt{2}\ln(\sigma_f)))^2) + ((1-P)/\ln(\sigma_c)) \exp(-((\ln(2r_i)-\ln(D_c))/(\sqrt{2}\ln(\sigma_c)))^2\} \quad (5)$$

Deposition Velocity

Deposition velocity (u) is defined as the flux to the surface (Jo) divided by concentration (c) measured at some distance from the surface (z). In dimensionless terms:

$$u^+c^+ = 1 \quad (6)$$

where $u^+ = u/v^*$

$c^+ = v^*c/Jo$

v^* = "friction velocity" = $\sqrt{\tau_o/\rho}$

τ_o = surface shear stress

ρ = air density

The term, c^+, is a "resistance" integral from the solution of a mass transfer equation for turbulent flow. In dimensionless terms, this solution is analogus to the solutions of similar momentum and heat transfer equations (4). Various forms of the "resistance" integral have been used to describe the deposition behavior of particles (5-16). There are four primary mechanisms of transport; 1) Brownian diffusion, 2) eddy diffusion, 3) inertial diffusion,

and 4) gravitational settling. Other forces that contribute to particle deposition are electrostatic charges, thermal gradients, mass attraction, and the condensation and evaporation of moisture. Three of the mechanisms (Brownian, eddy, and inertial diffusion) are included in the "resistance" integral c^+. Gravitational settling is not a function of change in concentration with distance from the surface and is not included in the integral.

Brownian Diffusion

Brownian diffusion is an extension of molecular diffusion theory to particles larger than molecules. When Brownian diffusion is the controlling mechanism, the "resistance" integral is directly proportional to the Schmidt number (Sc) for particles. The Schmidt number (Sc) is a function of particle radius and fluid viscosity. Values can be obtained from tables or calculated using equations (16).

Eddy Diffusion

Eddy diffusion is the result of the turbulent movement of the fluid and is the same as eddy viscosity. Thus, the form and magnitude of eddy diffusivity can be determined from momentum transport data. The most extensive set of such data are the work of Nikuradse (4). The eddy diffusivity function was obtained by best fitting numerial integrations to the Nikuradse Reynolds Number (RE) - friction factor (f) data for flow in both smooth and rough surface pipes. It is primarily a function of the distance from the surface and the surface roughness.

Inertial Diffusion

Particle inertia can increase or decrease the flux of particles to the surface depending on size. Within the particle size range where inertial diffusion is the controlling mechanism, the flux of smaller particles is increased by inertia while the flux of larger particles is decreased. In-

creased fractional penetration of the boundary layer with increased particle size does not compensate for the reduced rate of transport in the turbulent core (5).

Inertial diffusivity is a function of Stokes number (τ^+) which may be obtained from tables or calculated from equations (7). The best data observing inertial effects were obtained by Liu and Agarwal (8). By best fitting numerical integrations (using the previously obtained functions for Brownian and eddy diffusivity) to these data, a function for inertial diffusivity was obtained. The resulting fit of the data is shown in Figure 1.

The "resistance" integral used to fit the data of Liu and Agarwal is applicable to smooth vertical surfaces. Surface roughness and gravitational settling to horizontal surfaces are additional important factors.

Surface Roughness

The major effect of surface roughness is to increase the friction velocity (v^*) by increasing the sheer stress at the surface (τ_o). Hahn, et al. (13), however, uses a theory that also predicts that in the Brownian diffusion controlled particle size range the dimensionless deposition velocity is inversely proportional to the one-fourth power of the dimensionless surface roughness height (h^+).

$$h^+ = hv^*/\nu \qquad (7)$$

where h is surface roughness height

ν is kinematic viscosity of fluid

Actual to apparent surface area ratio due to surface roughness could also affect deposition velocity.

Friction Velocity. Buildings are perturbances in a larger flowing mass of air. With respect to deposition of particles to flat surfaces on buildings,

the friction velocity of interest is the one associated with those surfaces and not the friction velocity associated with the air mass in general.

The velocity of a fluid at the surface of a flat plate parallel to the flow is zero and increases with distance from the surface until it is the same as the main stream. Theoretically, this boundary layer thickness is infinite. "Usually, the edge of the boundary layer is defined as the point where the velocity reaches some fraction, say .99, of the mainstream velocity" (4). The theory associated with this boundary layer can be used to calculate friction velocity (v^*).

$$v^* = v_A \sqrt{f/2} \tag{8}$$

where v_A = mainstream velocity (wind speed)

f = friction factor

From boundary layer theory (4), the friction factor changes with surface size and roughness projected into the flowing air stream. It can be approximated for flat surfaces by:

$$f = 0.03/(RE_L)^{1/7} + 0.1(h/L)^{1/3} \tag{9}$$

where $RE_L = Lv_A/\nu$ = Reynolds Number

L = length of surface over which the air flows

h = height of surface roughness

Table 1 is an example of friction velocities over one meter of various surfaces at different windspeeds as calculated using these relationships. Similar equations and calculations could be applied to other shapes and orientations.

Gravitational Settling

Gravitational settling to horizontal surfaces is a function of the concentration and the terminal settling velocity of a specific size particle.

The terminal settling velocity can be obtained from tables or calculated using Stoke's law.

The dimensionless deposition velocity to a horizontal surface (floor) (u_h^+) is a function of the "resistance" integral (c^+) for a vertical surface and the dimensionless terminal settling velocity ($v_T^+ = v_T/v^*$)(10).

$$u_h^+ = v_T^+/(1-\exp(-v_T^+c^+)) \tag{10}$$

Simplified Deposition Velocity Model

The theoretical model for deposition velocity requires numerical integration because it is so complex. This was done for wide range of conditions of particle size and density, surface roughness, and friction velocity for both vertical and horizontal surfaces. It was apparent from these results that the effects of some mechanisms were negligible for certain particle size ranges and that the deposition velocity could be approximated very well by empirical additive deposition velocities for primary mechanisms. For smaller particle diameter the effects of inertia are negligible. For larger particles inertial diffusion is the primary mechanism. Even larger partilces are controlled only by eddy diffusion.

Brownian Diffusion Region

In the region where only Brownian and eddy diffusion are important factors, the theoretical curves fit empirical straight lines in log-log form resulting in the following equation:

$$u_B^+ = 1/(7.4\times10^8(r^+/v^*)^{1.13}(1+h^+/16)^{0.25}) \tag{11}$$

where u_B^+ = dimensionless deposition velocity in the Brownian diffusion region

r^+ = dimensionless particle radius = rv^*/ν

ν = kinematic viscosity

Inertial Diffusion Region

In this region the dimensionless deposition velocity (u_i^+) is a function of the Stoke's number (τ^+). The deposition velocity increases as the squares of the Stoke's number increases up to a certain point where it begins to decrease. The empirical fit of the theoretical curve in this region gives the following equation:

$$u_i^+ = 0.0005\tau^+(0.5 + \tau^+)(1-\exp(-(17.6/\tau^+)^{2.5})) \quad (12)$$

Eddy Diffusion Region

For the largest particles, eddy diffusion is the controlling mechanism. The dimensionless deposition velocity (u_e^+) is a function of particle radius and the distance from the surface where the concentration is measured (z_c^+)

$$u_e^+ = 1/(100/r^{+2}+3.3\ \ln(z_c^+/r^+)) \quad (13)$$

Agreement with Available Data

The summation of Equations 11, 12, and 13 is a close approximation of the inverse of the "resistance" integral (c^+). It is much easier to use and less time consuming than numerical integration.

Based on available data (8)(9)(10)(12)(13)(14)(15)(16) presented in Figure 2 there appears to be a minimum deposition velocity of around 5×10^{-3} cm/sec which is greater than a minimum predicted by the summation of the above contributions and gravitational settling. Electrostatic forces, thermal forces, mass attraction, and condensation and evaporation of moisture can all contribute to this minimum. In dimensionless terms:

$$u_m^+ = .005/V^* \quad (14)$$

To vertical surfaces:

$$u^+ = u_B^+ + u_e^+ + u_i^+ + u_m^+ \quad (15)$$

and to upper horizontal surfaces

$$u_H^+ = V_T^+/(1-\exp(-V_T^+/u^+)) \quad (16)$$

The data in Figure 2 represents a wide range of conditions; vertical and horizontal surfaces, smooth and very rough surfaces, tubes and plates, and friction velocities from 14 cm/sec to 316 cm/sec. There is, however, only about a two order of magnitude range for any one dimensionless particle radius. The data of Hahn et al. (13) indicate that the range for any one set of conditions is around an order of magnitude. The two curves on Figure 2 represent the predictions of Equations 15 and 16 for extreme conditions. The theoretical predictions are consistent with the measured values and are well within experimental error.

APPLICATION OF MODEL

Concentration of different size particles as described by Equation 5 and deposition velocity as a function of particle size given by Equations 11 through 16 are the complex components in the model for soiling potential (Equation 3). The other factors are not complex.

Soiling Potential

The transition particle radius (r_t) in Equation 4 (that changes units of volume to area with increasing particle radius) is assumed to be 0.1μ. If the units of particle radius (r_i) is in micrometers, the concentration (c_i) is $\mu g/m^3$, friction velocity (v^*) is cm/sec, and the particle density ρ_p is gm/cm^3 the constant α is 0.315. The resulting equation for soiling potential (k_i) as a function of particle size is:

$$k_i = 0.315 c_i u_i^+ v^* / [\rho_p (r_i^+ + 0.075/(0.1 + r_i))] \qquad (17)$$

where k_i is per year

Figure 3 shows the effects of surface roughness, orientation, and windspeed on the soiling potential of different particle sizes. The total concentration is 100 $\mu g/m^3$ with 75% in the fine mode. The mass median

diameters for the two modes are 0.4 μm and 10 μm with a geometric standard deviation of 2 for both. The particle density is 1 gm/cm^3.

At these windspeeds, changing the variables has little effect on the soiling potential of the fine particles. The effects, however, are dramatic for the coarse particles. Gravitational settling is dominant at a windspeed of 3 m/sec. For the vertical surface at this windspeed, surface roughness makes a significant contribution. At 6 m/sec, inertial diffusion becomes the dominant deposition mechanism in the coarse mode for all surfaces.

The total soiling potential for this distribution of particles is $K = \Sigma k_i$. Table 2 summarizes the results pictured in Figure 3. Also included are the contributions to soiling potential of fine and coarse particles and those particles collected by a PM10 measuring device (designed to collect particles with diameters less than 10μ). It should be noted that about 85 percent of this distribution is below 10 μm yet the soiling potential for these particles varies from 26 to 88 percent of the total depending on the set of conditions. Thus, PM10 alone is not a good proxy for soiling potential.

Change in Reflectance as a Function of Time

By assuming values for the reflectance of the substrate and particles these soiling potentials can be used in Equations 1 and 2 to show how various conditions affect soiling at a particular ambient particle distribution. Figure 5 presents the results assuming the substrate reflectance (R_o) is 90 percent and the particle reflectance is 30 percent.

CONCLUSIONS

Soiling of surfaces by airborne particles can be predicted from theoretical relationships. Reflectance change is related to the accumulation of particles on a surface. The flux to the surface is dependent on ambient concentration and deposition velocity, both of which are particle size dependent. A bimodal log normal model for size distribution of concentration combined with summations of contributions of Brownian, eddy, and inertial diffusion form the basis of a flux relationship.

The greatest effect of surface roughness on deposition velocity is by changing the friction velocity (V^*). Based on boundary layer theory, friction velocity can be predicted from windspeed, size of surface, and height of surface roughness.

The ambient measurement of any size fraction of particles, by itself, is not a good proxy of soiling potential. Soiling varies considerably with windspeed, surface orientation and roughness.

REFERENCES

1. Haynie, F., and J. Spence, Chairman, "Final Report of the EPA Workshop on Research Strategies to Study the Soiling on Buildings and Materials." Environmental Sciences Research Laboratory, U.S. EPA, Research Triangle Park, NC, April 1984, 50 pp.

2. Lundgren, D.A., and H. J. Paulus, "The Mass Distribution of Large Atmospheric Particles," Journal of the Air Pollution Control Association, 25, No. 12, 1227-1231, (1975) December.

3. Watson, J. G., J. C. Chow, J. J. Shah, and T. G. Pace, "The Effect of Sampling Inlets on the PM-10 and PM-15 to TSP Concentration Ratios," Journal of the Air Pollution Control Association, 33, No. 2, 114-119, (1983) February.

4. Knudsen, J. G., and D. L. Katz, "Fluid Dynamics and Heat Transfer," Engineering Research Bulletin, No. 37, University of Michigan Press, Ann Arbor, Michigan, 1954, 243 pp.

5. Reeks, M.W., and G. Skyrme, "The Dependence of Particle Deposition Velocity on Particle Inertia in Turbulent Pipe Flow," Journal of Aerosol Science, 7, 485-495 (1976).

6. Browne, L.W.B., "Deposition of Particles on Rough Surfaces During Turbulent Gas-Flow in a Pipe," Atmospheric Environment, 8, 801-816 (1974).

7. Wood, N.B., "A Simple Method for the Calculation of Turbulent Deposition to Smooth and Rough Surfaces," Journal of Aerosol Science, 12, No. 3, 275-290 (1981).

8. Liu, B.Y.H., and J. K. Agarwal, "Experimental Observation of Aerosol Deposition in Turbulent Flow," Journal of Aerosol Science, 5, 145-155 (1974).

9. Clough, W.S., "Transport of Particles to Surfaces," Aerosol Science, 4, 222-234 (1973).

10. Sehmel, G.A., "Particle Eddy Diffusivities and Deposition Velocities for Isothermal Flow and Smooth Surfaces," Aerosol Science, 4, 125-138 (1973).

11. El-Shobokshy, M.S., and I.A. Ismail, "Deposition of Aerosol Particles from Turbulent Flow onto Rough Pipe Wall," Atmospheric Environment, 14, 304 (1980).

12. Sehmel, G.A., W. H. Hodgson, and S. L. Sutter, "Dry Deposition of Particles," Pacific Northwest Laboratories Annual Report for 1973, BNWL-1850 PT3, Battelle, Richland, WA, April 1974, pp. 157-162.

13. Hahn, L.A., J. J. Stukel, K. H. Leong, and P. K. Hopke, "Turbulent Deposition of Submicron Particles on Rough Wall," Journal of Aerosol Science, 16, No. 1, 81-86 (1985).

14. Lane, D. D., J. J. Stukel, "Aerosol Deposition on a Flat Plate," Journal of Aerosol Science, 9, 191-197 (1978).

15. Sehmel, G.A. and S. C. Sutter, "Particle Deposition Rates on Water Surface as a Function of Particle Diameter and Air Velocity," Journal de Recherches Atmospheriques, 8, No. 3-4, 911-920 (1974).

16. Wildi, J., and H. Thomann, "Measurement of the Deposition Velocity of Small Particles in Stationary and Oscillating Turbulent Pipe Flow," Journal of Aerosol Science, 14, 615-632 (1983).

Table 1. Calculated Friction Velocities for Different One Meter Surfaces and Windspeeds - cm/sec

Surface	Roughness Height cm	Windspeed - m/sec 3	6	12
Glass	0	15.4	29.2	55.7
Flat Paint	.01	21.1	41.1	80.3
Concrete	0.1	26.2	51.5	101.5
Gravel	1	34.7	68.8	136.4

Table 2. Soiling Potentials as a Function of Surface Roughness, Windspeed, and Orientation

Windspeed-m/sec	Orientation	Glass				Flat Paint			
		Fine	PM10	Coarse	Total	Fine	PM10	Coarse	Total
3	Vertical	0.257	0.264	0.042	0.300	0.267	0.277	0.125	0.392
	Horizontal	0.244	0.405	0.669	0.964	0.304	0.414	0.683	0.987
6	Vertical	0.284	0.305	0.381	0.665	0.309	0.385	1.100	1.419
	Horizontal	0.321	0.432	0.836	1.157	0.345	0.490	1.501	1.846

Particle Distribution: 100 $\mu g/m^3$ Total, 75% fine, modes 0.4 μ and 10 μ

$\sigma_f = \sigma_c = 2$

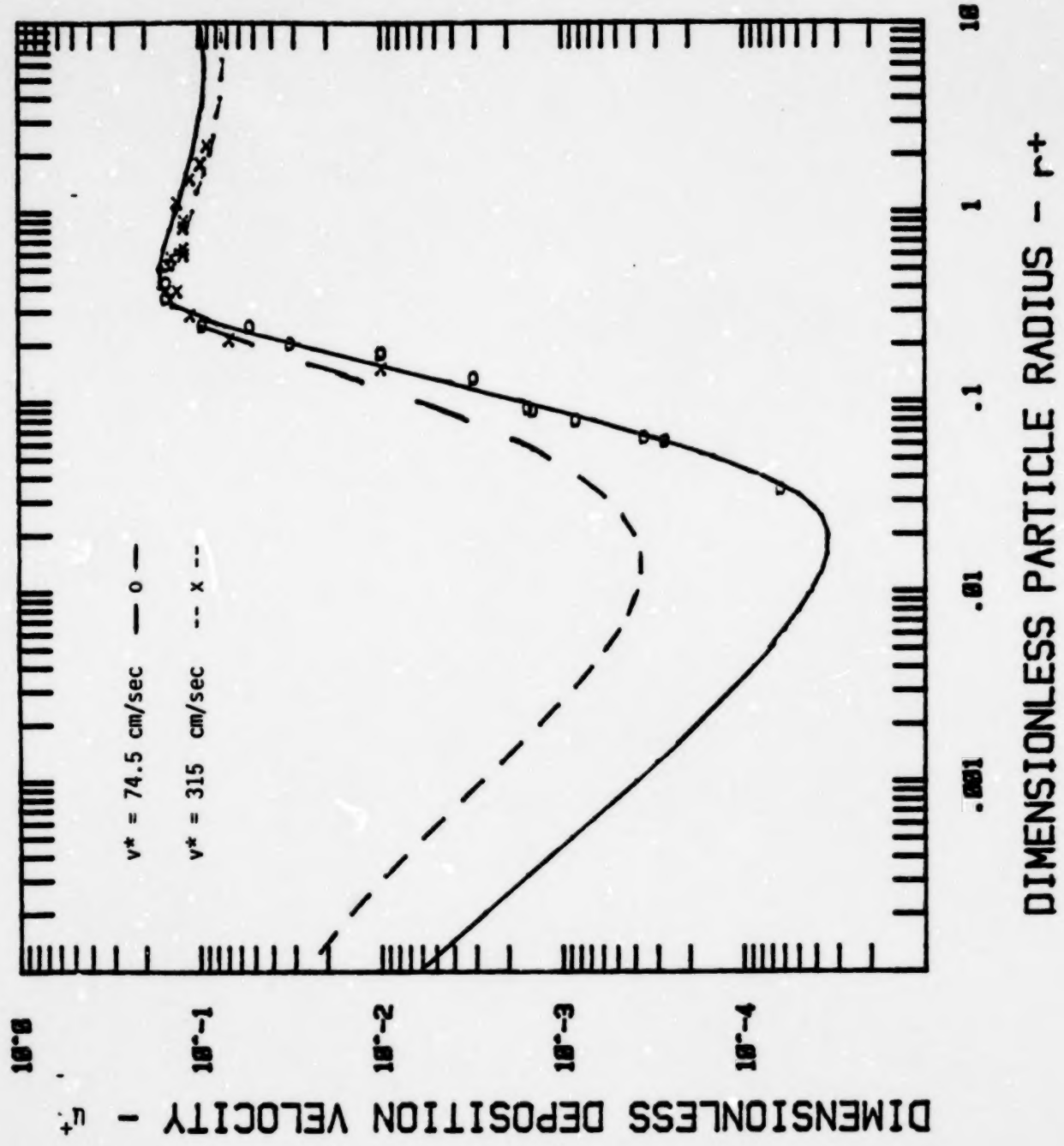

Figure 1. Theoretical fit of data of Liu and Agarwal (8).

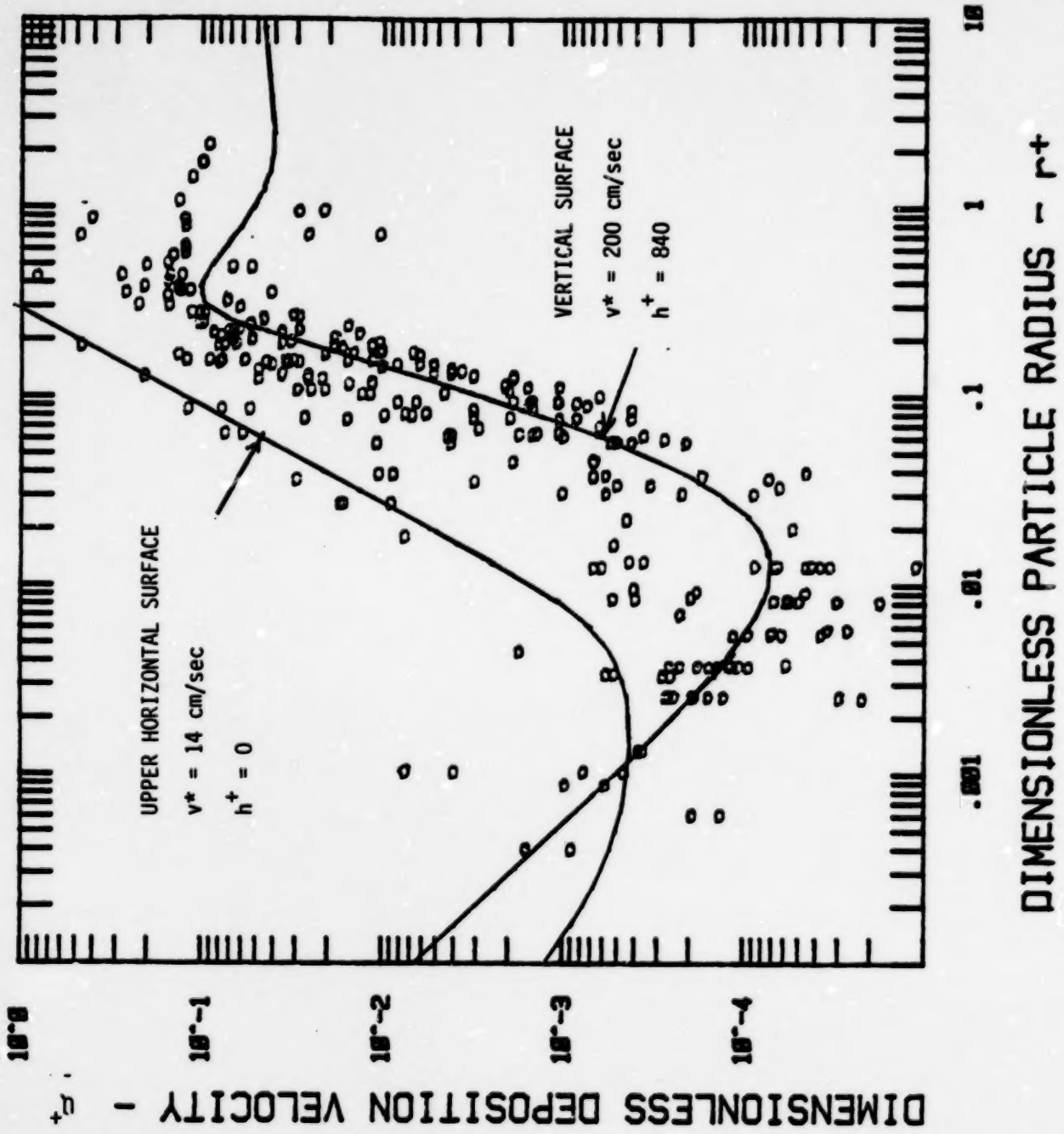

Figure 2. Theoretical curves compared with data for a wide-range of conditions (8-10, 12-16).

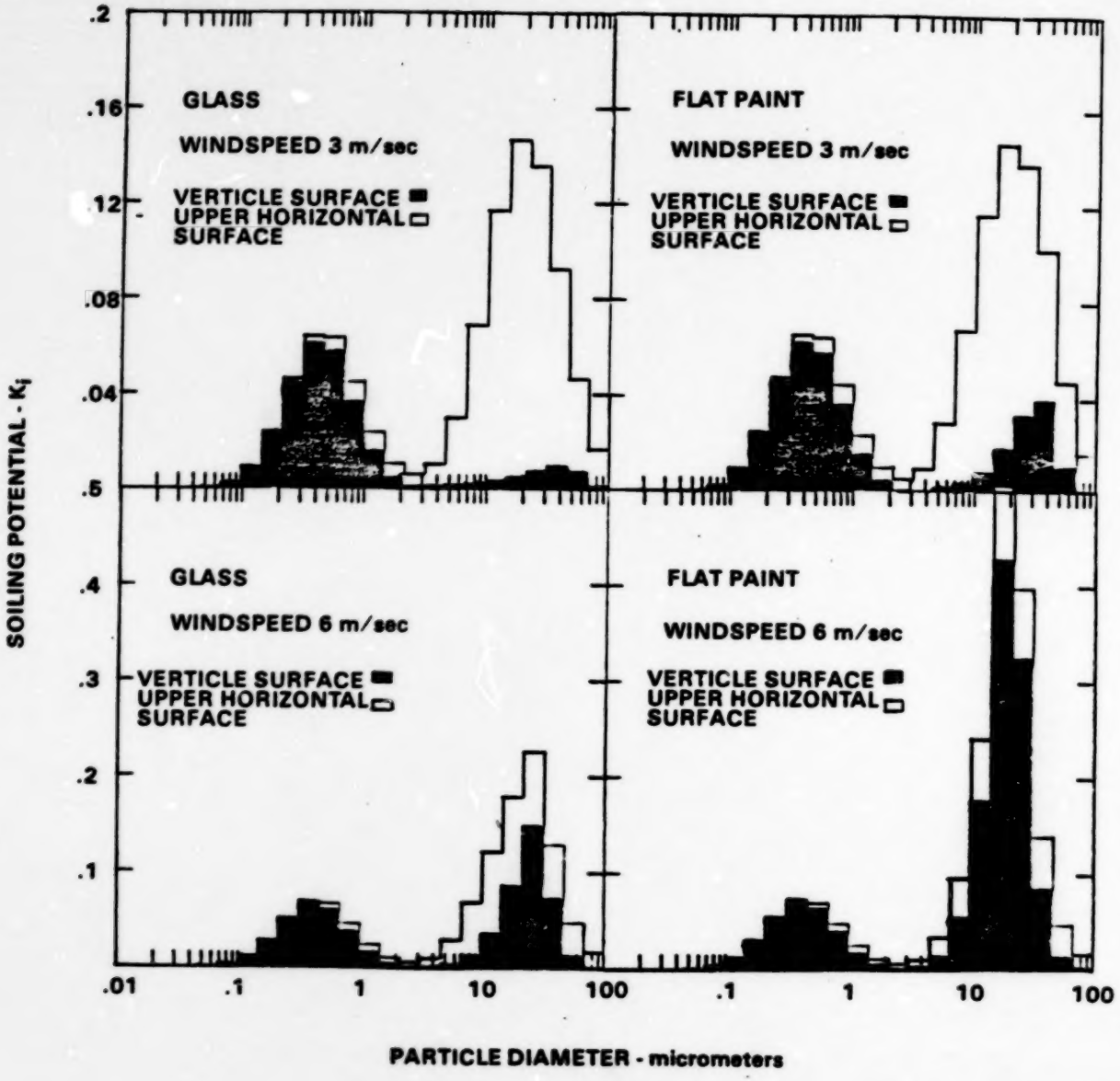

Figure 3. Soiling potential as a function of particle diameter for different surfaces and windspeeds (see text for particle size distribution).

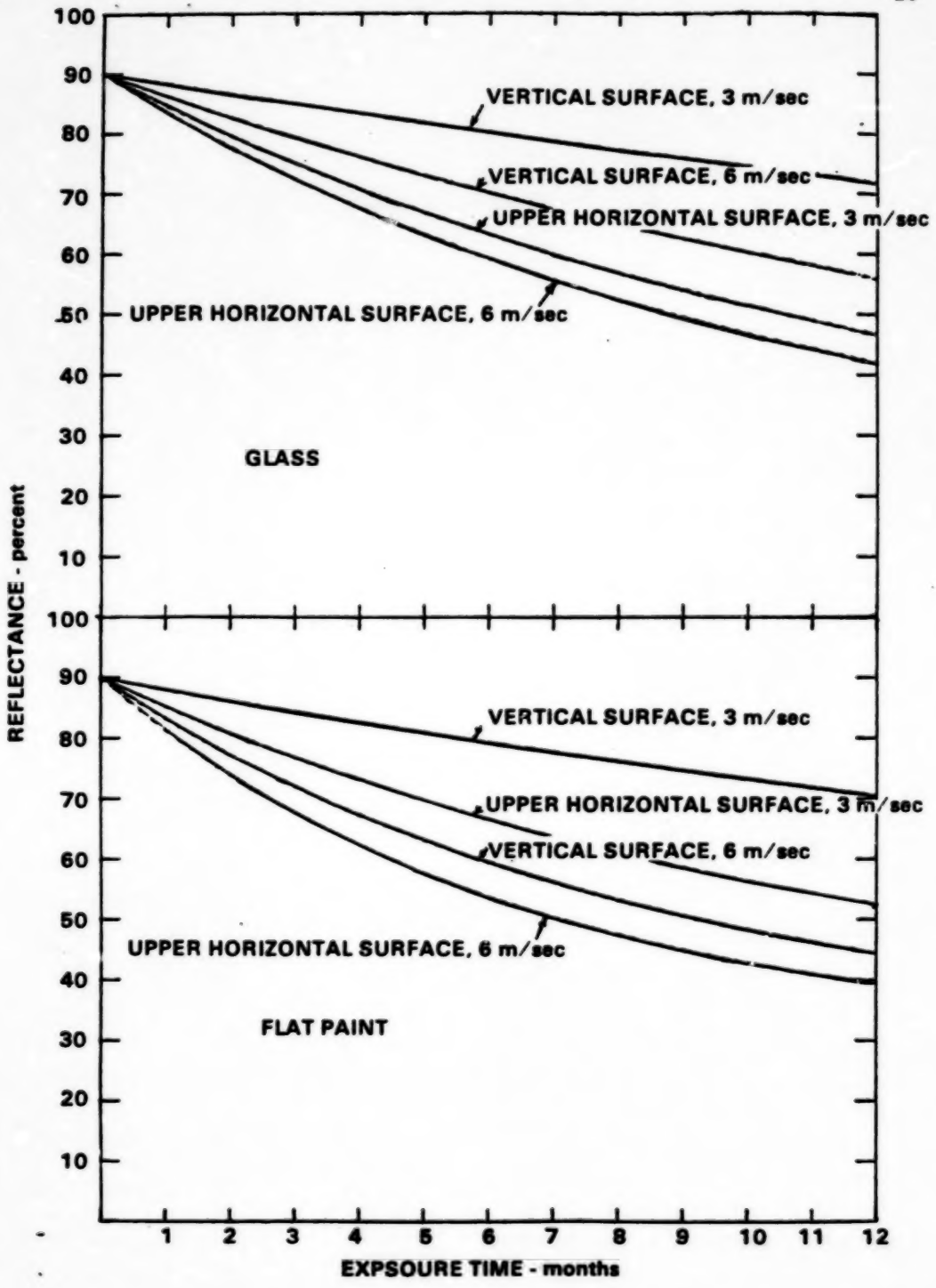

Figure 4. Reflectance change with time for different surfaces and windspeeds; substrate reflectance (R_O) = 90%, particle reflectance (R_p) = 30%, values of soiling potential (k) from Table 2.